

Resonance poles and threshold energies for hadron physical problems by a model-independent universal algorithm

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Abstract

We show how complex resonance poles and threshold energies for systems in hadron physics can be accurately obtained by using a method based on the Padé-approximant which was recently developed for the calculation of resonance poles for atomic and molecular auto-ionization systems. The main advantage of this method is the ability to calculate the resonance poles and threshold energies from *real* spectral data. In order to demonstrate the capabilities of this method we apply it here to an analytical model as well as to experimental data for the squared modulus of the vector pion form factor, the S0 partial wave amplitude for $\pi\pi$ scattering and the cross section ratio $R(s)$ for e^+e^- collisions. The extracted values for the resonance poles of the $\rho(770)$ and the $f_0(500)$ or σ meson are in very good agreement with the literature. When the data are noisy the prediction of decay thresholds proves to be less accurate but feasible.

Keywords: Resonance poles, threshold energies, Padé approximant, analytic continuation

1. Introduction

The determination of resonance poles, uniquely defined as poles of the S -matrix in the complex energy plane, is a long-standing problem and particularly difficult for broad resonances or if decay channels open up in the vicinity. In these cases, simple approaches like a standard Breit-Wigner parametrization fail and more involved theoretical tools like dispersive approaches are necessary, see e.g. [1] for reviews. However, these rigorous analytic methods require powerful mathematical techniques which makes them complicated to use in many cases.

In this letter we introduce a method that was originally developed for the calculation of auto-ionization resonances in quantum chemistry [2–4] to the field of hadron physics. This method is based on the Padé-approximant, model-independent, easy to use and has a broad range of applicability. In contrast to other methods, see e.g. [5], it only requires a set of real data points as input from which information on the complex plane can be extracted by performing an analytic continuation. We wish to refer to this method as Resonances Via Padé (RVP) method.

In order to demonstrate this method we will apply it here to an analytical model as well as to experimental data for different observables in order to extract the locations of resonance poles and decay thresholds. We believe that the method represents a viable tool to study the analytic properties of a function given only in numerical form and that it can be used together with existing methods in a large range of situations, including the determination of resonance poles.

This letter is organized as follows: In Sec. 2 we review the RVP method which is based on the Padé approximant and was

recently developed for calculating auto-ionization resonance poles. In Sec. 3 we apply it to an analytical model for the spectral density function of some hypothetical particle in order to extract the locations of the resonance pole and the decay thresholds. In Sec. 4 the method is then applied to experimental data on the squared modulus of the vector pion form factor, $|F_\pi|^2$, in order to extract the resonance pole location of the charged $\rho(770)$ meson. In Sec. 5 the method is applied to the S0 partial wave amplitude for $\pi\pi$ scattering and the location of the σ -meson pole is extracted. In Sec. 6 we use data on the cross section ratio $R(s)$ for e^+e^- collisions and discuss the possibility to predict the charm quark production threshold. We summarize and conclude in Sec. 7.

2. Resonances Via Padé (RVP) method

Recently, among the computational chemistry community, there has been a growing interest in the calculations of complex poles of atomic and molecular scattering matrices by using *real computational* results [2–4, 6–8]. In these calculations, one first constructs a function $F(\eta)$ based on real data points η_i and then performs an analytic continuation to the complex plane by allowing for complex arguments η . In the following we will adapt the Padé-approximant approach suggested by Landau et al. [2, 4]. This approach avoids the need to calculate higher-order derivatives as necessary for a Taylor expansion series or other methods which use the Padé-approximant [5].

The aim is to find a function $F(\eta)$ which represents the correct analytic continuation based on the real values of input

points. This function is expressed as a ratio of two polynomials,

$$F(\eta) = \frac{P(\eta)}{Q(\eta)}. \quad (1)$$

When given a finite set of M data points (η_i, F_i) , it is in general not possible to find $F(\eta)$ exactly. We will therefore construct an analytical approximation to $F(\eta)$ by using the Schlessinger point method [9]. The Schlessinger truncated continued fraction $C_M(\eta)$ is then given by

$$C_M(\eta) = \frac{F(\eta_1)}{1 + \frac{z_1(\eta - \eta_1)}{1 + \frac{z_2(\eta - \eta_2)}{\ddots z_M(\eta - \eta_M)}}}, \quad (2)$$

where the z_i are real coefficients chosen such that

$$C_M(\eta_i) = F(\eta_i), \quad i = 1, 2, \dots, M. \quad (3)$$

Once the z_i are determined, an analytic continuation into the complex plane is performed by choosing η to be complex, i.e. $\eta = ae^{i\theta}$. For further details on this method and the numerical implementation we refer to [2, 4].

3. Analytical example

In order to demonstrate and test the capabilities of the RVP method described in the previous section, we will apply it first to an analytical model. We choose the model to be for the spectral density function, or spectral function, of some hypothetical particle but stress that the method can also be applied to various other quantities such as form factors or scattering amplitudes, as demonstrated in the following sections.

The model for the spectral function is given by

$$\rho(\omega^2) = -\frac{1}{\pi} \text{Im} \left(\frac{1}{\omega^2 - M^2 - \Pi(\omega^2)} \right) \quad (4)$$

with the self energy

$$\Pi(\omega^2) = S_1 \log(T_1^2 - \omega^2) + S_2 \log(T_2^2 - \omega^2) \quad (5)$$

and parameters $M = 50$ MeV, $S_1 = 2000$ MeV, $T_1 = 0$ MeV, $S_2 = 3000$ MeV, $T_2 = 300$ MeV. When evaluated for real energies, ω is understood to represent the retarded limit, i.e. $\omega \rightarrow \omega + i\varepsilon$ with $\varepsilon \rightarrow 0$. The spectral function is antisymmetric, $\rho(\omega) = -\rho(-\omega)$, and correctly normalized,

$$\int_0^\infty \rho(\omega^2) d\omega^2 = 1. \quad (6)$$

The resulting spectral function is shown in Fig. 1 and describes a single resonance as well as two decay channels. The decay channels arise from the logarithmic branch cuts of the self energy $\Pi(\omega^2)$ and open at T_1 and T_2 . The complex pole associated to the resonance peak is located on the second Riemann sheet (2RS) and can be found numerically by solving $\omega_p^2 - M^2 - \Pi_{2RS}(\omega_p^2) = 0$ for complex ω_p . The self energy on the second Riemann sheet, Π_{2RS} , can be straightforwardly obtained

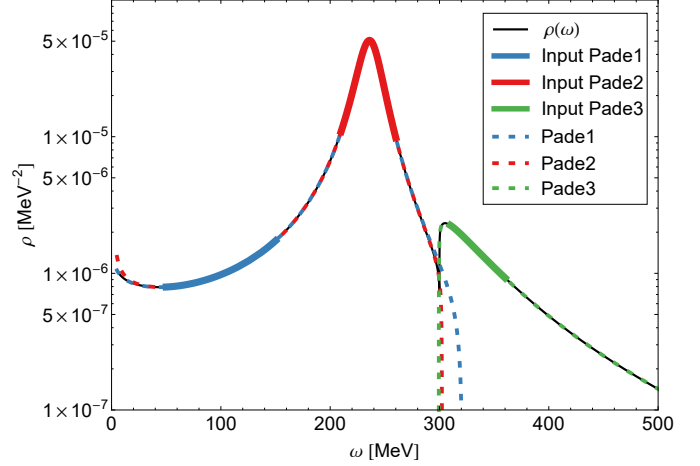


Figure 1: (color online) The spectral function defined in Eq. (4) is shown together with three different input regions for the RVP method and the corresponding extrapolations. It describes a single resonance peak in the vicinity of two decay thresholds at $T_1 = 0$ MeV and $T_2 = 300$ MeV. The input regions 1 and 2 can be used to identify the complex pole associated to the resonance peak as well as the decay thresholds T_1 and T_2 while input region 3 can be used to describe the spectral function for $\omega > T_2$ and to identify T_2 .

from Eq. (5) by using that the discontinuity along the branch cut of the complex logarithm is given by $i2\pi$, which gives

$$\Pi_{2RS}(\omega^2) = S_1 (\log(T_1^2 - \omega^2) - i2\pi) + S_2 \log(T_2^2 - \omega^2). \quad (7)$$

The complex pole associated to the resonance peak is then found to be at $\omega_p \approx (236.43 - i12.64)$ MeV.

We will now apply the RVP method to this model in order to extract the location of the complex pole as well as the locations of the decay thresholds using only real numerical data generated by Eq. (4) as input. We use data points from three different ω -regimes as input which are shown in Fig. 1.

The first two input regimes are chosen between the two decay thresholds, T_1 and T_2 , and therefore lie in the same analytic regime of the spectral function. Both can be used to reconstruct the spectral function in this regime as well as to determine the location of the thresholds and of the complex pole associated to the resonance.

From the first input region we find the lower threshold at $T_1^{\text{Pade1}} \approx -2$ MeV and the upper threshold at $T_2^{\text{Pade1}} \approx 329$ MeV while we find $T_1^{\text{Pade2}} \approx 0$ MeV and $T_2^{\text{Pade2}} \approx 303$ MeV from the second input region. The fact that the upper threshold T_2 can be correctly identified by using input points below that threshold is remarkable. Whether thresholds can also be ‘predicted’ when using (noisy) experimental data as input will be discussed in Sec. 6. When using the third input region beyond the second threshold, we are able to reconstruct the spectral function in this analytic regime and find $T_2^{\text{Pade3}} \approx 299$ MeV for the location of the second threshold. We note that each input region can be used to identify the thresholds adjacent to it and well describe the spectral function in between these thresholds. Furthermore, it is even possible to describe the structure of the spectral function beyond these thresholds, but with less accuracy [2, 4].

The functions generated from the first two input regions can also be used to locate the complex resonance pole by allow-

ing for complex arguments. Remarkably, both yield the same result, i.e. $\omega_p^{Pad\acute{e}1, Pad\acute{e}2} \approx (236.43 - i12.64)$ MeV. The difference between this and the correct result is negligible and can be viewed as the theoretical error of the RVP method, which in the present case is smaller than 0.01 MeV.

4. Complex pole of the charged $\rho(770)$ meson

In this section we will use the RVP method to analyze the ALEPH data on the squared modulus of the $\pi^-\pi^0$ vector form factor $|F_\pi(s)|^2$ [10, 11]. These data were obtained from τ -lepton decays, $\tau^- \rightarrow \pi^-\pi^0\nu_\tau$, and represent the cleanest determination of the $\rho(770)$ -meson mass and width.

In Fig. 2 we show the experimental data on the pion form factor $|F_\pi(s)|^2$ from [11] together with the input range chosen for the RVP method and the resulting extrapolation function. The input range was chosen around the resonance peak at $s \approx 0.6$ GeV² and $M = 30$ input points were used. By studying the extrapolation function for complex arguments we find the complex pole of the charged $\rho(770)$ meson to be at $\sqrt{s_\rho} = M_\rho - i\Gamma_\rho/2$ with

$$M_\rho = 761.8 \pm 1.9 \text{ MeV}, \quad \Gamma_\rho = 139.8 \pm 3.6 \text{ MeV}. \quad (8)$$

The errors represent the total (experimental and theoretical) uncertainties. The experimental uncertainties were obtained by extracting the complex pole not only from the central values but also from the upper and lower values for $|F_\pi(s)|^2$, cf. Fig. 2. The theoretical error from the RVP method has been estimated by changing the number of input points, which corresponds to changing the order of the Padé approximant, and is found to be of the order 0.002 MeV, i.e. negligible compared to the experimental uncertainties.

The averaged values for the charged $\rho(770)$ meson are listed as $M_\rho = 775.11 \pm 0.34$ MeV and $\Gamma_\rho = 149.1 \pm 0.8$ MeV in the 2015 Review of Particle Physics (RPP) [1]. However, these

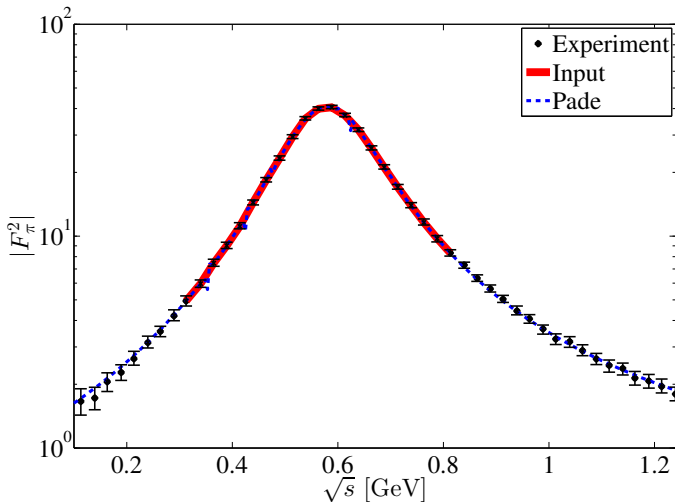


Figure 2: (color online) Experimental data for the squared modulus of the pion form factor $|F_\pi(s)|^2$ from [11] together with the input range chosen for the RVP method (solid red) and the corresponding extrapolation function (dashed blue).

M_ρ (MeV)	Γ_ρ (MeV)	source
762.5 ± 2	142 ± 7	[12]
758.3 ± 5.4	145.1 ± 6.3	[13]
$764.1 \pm 2.7^{+4.0}_{-2.5}$	$148.2 \pm 1.9^{+1.7}_{-5.0}$	[14]
754 ± 18	148 ± 20	[15]
763.0 ± 0.2	139.0 ± 0.5	[16]
760 ± 2	147 ± 6	[17]
761 ± 1	139 ± 2	[18]
763.7 ± 1.2	144 ± 3	[19]
761.8 ± 1.9	139.8 ± 3.6	this work

Table 1: Collection of pole parameter predictions for the $\rho(770)$ meson.

parameters are usually obtained from generalized Breit-Wigner formulas and are not to be confused with the coordinates of the complex pole in the S or T matrix. We therefore have to compare our result for the pole position to other predictions for the resonance pole from the literature and find very good agreement, see Tab. 1.

We stress again that the employed RVP method only requires real data as input, in this case for the pion form factor $|F_\pi(s)|^2$, without any need for information on the imaginary part of the form factor such as the $\delta_1^1(s)$ phase shift, in contrast to other methods, see e.g. [5]. We also note that, in general, one finds more than one pole when using the RVP method. These additional poles are unphysical and can easily be identified by changing the input regime or the number of input points. Only the coordinates of the physical pole (and its mirror pole with positive imaginary part) remains unaffected by these modifications which allows for a unique determination.

5. Complex pole of the $f_0(500)$ - or σ meson

The identification of scalar mesons and their resonance poles is a long-standing puzzle and particularly difficult for the $f_0(500)$ or σ meson due to its large decay width and the strong overlap with the background and higher resonances. For a review on the history and the current status of the σ meson we refer to [20].

In the following we will apply the RVP method the S_0 partial-wave amplitude as obtained from the Constrained Fit to Data (CFD) parametrization of the $\delta_0^{(0)}(s)$ phase shift provided in [21] which is based on experimental data on $K_{\ell 4}$ decays [22], in particular the final data from NA48-2 [23], and a selection of existing $\pi\pi$ scattering data (see [21] for details).

Following [21], the partial-wave amplitude for $\pi\pi$ scattering in the $IJ = 00$ channel is given by

$$t_0^0(s) = \frac{\eta_0^0(s)e^{2i\delta_0^0(s)} - 1}{2i\rho_\pi(s)}, \quad (9)$$

with the phase space factor

$$\rho_\pi(s) = \sqrt{1 - 4M_\pi^2/s} \quad (10)$$

and the inelasticity $\eta_0^0(s) = 1$ for the energy range considered here. The CFD parametrization for the phase shift $\delta_0^{(0)}(s)$ reads

$$\cot \delta_0^{(0)}(s) = \frac{s^{1/2}}{2k} \frac{M_\pi^2}{s - \frac{1}{2}z_0^2} \times \left(\frac{z_0^2}{M_\pi \sqrt{s}} + B_0 + B_1 W(s) + B_2 W(s)^2 + B_3 W(s)^3 \right) \quad (11)$$

with

$$W(s) = \frac{\sqrt{s} - \sqrt{s_0 - s}}{\sqrt{s} + \sqrt{s_0 - s}}, \quad s_0 = 4M_K^2, \quad (12)$$

and

$$k(s) = \sqrt{s/4 - M_\pi^2}. \quad (13)$$

The parameters used in these expressions are summarized in Tab. 2.

We will now apply the RVP method to the real part of the partial wave amplitude $t_0^0(s)$ as defined in Eq. (9). In Fig. 3 the real part of $t_0^0(s)$ is shown together with the input region used and the corresponding extrapolation function. We note that it is also possible to use other input regions to determine the complex pole of the σ meson since all input regions are generated by the same analytic function which can therefore be reconstructed from any region. In the following we will choose

B_0	B_1	B_2	B_3
7.14 ± 0.23	-25.3 ± 0.5	-33.2 ± 1.2	-26.2 ± 2.3

Table 2: Parameters for the CFD parameterization of the S0 wave phase shift data from [21]. In addition, the pion mass is set to $M_\pi = 139.57$ MeV, the kaon mass to $M_K = 496$ MeV and $z_0 = M_\pi$. We note that this parameterization is only valid up to $\sqrt{s} = 850$ MeV.

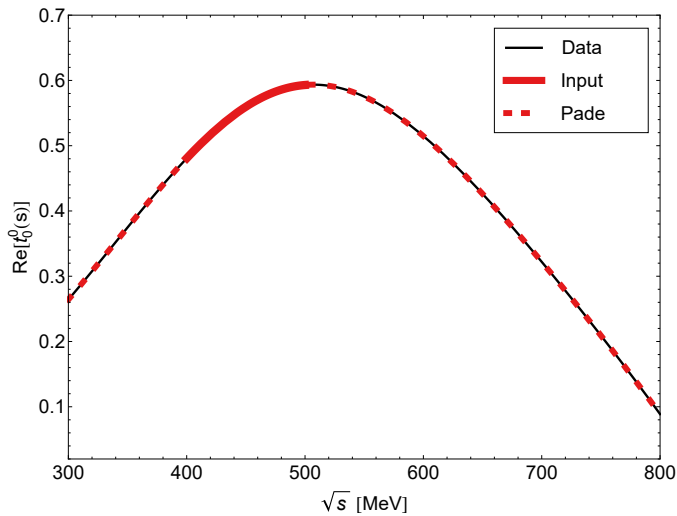


Figure 3: (color online) The real part of the S0 partial wave amplitude, $\text{Re}t_0^0(s)$, as obtained from the Constrained Fit to Data (CFD) parameterization of the $\delta_0^{(0)}(s)$ phase shift provided in [21] is shown together with the chosen input range for the RVP method as well as the obtained extrapolation.

input points from a region between $\sqrt{s} = 400$ and 500 MeV which is closest to the resonance pole in the complex energy plane.

We find the complex pole of the σ meson to be located at

$$\sqrt{s_\sigma} = 450.1 \pm 11.2 - i(299.2 \pm 12.2) \text{ MeV} \quad (14)$$

where the errors represent the total uncertainties which were obtained by determining the pole position not only for the central values of the parameters B_i from Tab. 2 but also for all possible combinations of their lower and upper values. The theoretical error from the RVP method is again negligible compared to the experimental uncertainties.

When compared to other predictions for the σ resonance pole we find excellent agreement, see Tab. 3. This comparison shows that our approach can compete with the most recent and advanced dispersive determinations.

$\sqrt{s_\sigma}$ (MeV)	source
$470 \pm 30 - i(295 \pm 20)$	[24]
$470 \pm 50 - i(285 \pm 25)$	[16]
$441_{-8}^{+16} - i(272_{-12.5}^{+9})$	[25]
$457_{-13}^{+14} - i(279_{-7}^{+11})$	[26]
$442_{-8}^{+5} - i(274_{-5}^{+6})$	[27]
$453 \pm 15 - i(297 \pm 15)$	[28]
$449_{-16}^{+22} - i(275 \pm 12)$	[20]
$450.1 \pm 11.2 - i(299.2 \pm 12.2)$	this work

Table 3: Collection of pole parameter predictions for the $f_0(500)$ or σ meson.

6. Prediction of decay thresholds for e^+e^- annihilation

As a final application of the RVP method we will use it to analyze data from e^+e^- collisions and discuss its ability to predict decay (or rather production) thresholds based on experimental data. In particular, we will analyze data on the ratio $R(s)$ between the total cross sections of e^+e^- into hadrons and into muons,

$$R(s) = \frac{\sigma(e^+e^- \rightarrow \text{hadrons})}{\sigma(e^+e^- \rightarrow \mu^+\mu^-)}, \quad (15)$$

where $\sigma(e^+e^- \rightarrow \text{hadrons})$ is the experimental cross section corrected for initial state radiation and electron-positron vertex loops, and $\sigma(e^+e^- \rightarrow \mu^+\mu^-) = 4\pi\alpha^2(s)/3s$ with the electromagnetic fine-structure constant $\alpha(s)$. Depending on the collision energy, different flavors of quarks can be produced.

A collection of data on the ratio $R(s)$ is shown in Fig. 4 together with two input regions used for the RVP method and the obtained extrapolation functions. We note that $R(s)$ exhibits a significant increase at $\sqrt{s} \approx 4$ GeV which is related to the production threshold of charm quarks, in particular of D mesons (see e.g. [29] for details). As shown in Fig. 4, only one of the Padé extrapolations correctly predicts a threshold at $\sqrt{s} \approx 4$ GeV while the other shows a smooth behavior.

The prediction of thresholds in this case has of course to be treated with care. First of all, the experimental data are noisy

which gives rise to a strong dependence on the chosen input points. Moreover, there are several smaller decay thresholds and resonance peaks present in the vicinity of the input regions chosen, which limits the radius of convergence of the obtained Padé extrapolations.

We therefore conclude that a robust prediction of decay thresholds is not possible in the present case. We note, however, that the RVP method discussed in this letter is in principle capable of predicting decay thresholds if the input is precise enough and if there is a sufficient number of input points available, as demonstrated for the analytical model in Sec. 3.

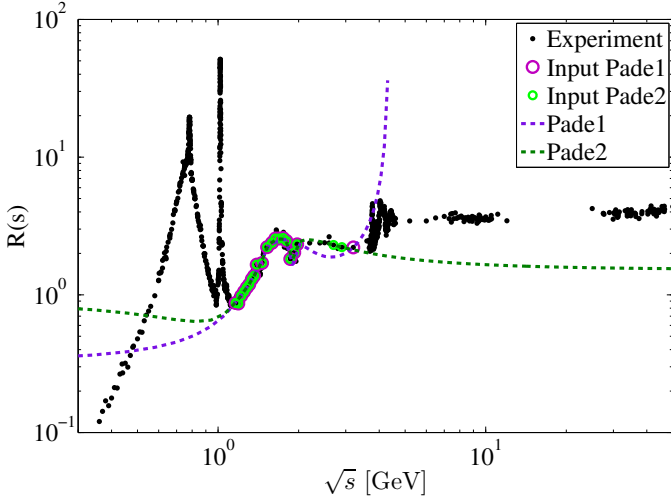


Figure 4: (color online) Collection of data on the ratio $R(s)$ between the total cross sections of e^+e^- into hadrons and into muons, $R(s) = \sigma(e^+e^- \rightarrow \text{hadrons})/\sigma(e^+e^- \rightarrow \mu^+\mu^-)$ from [1]. Also shown are two input regions chosen for the RVP method together with the resulting extrapolations.

7. Summary

In this letter we have introduced a method that was originally developed in [2–4] for the calculation of auto-ionization atomic and molecular resonances in quantum chemistry to hadron physics with the aim to identify resonance poles and to predict decay thresholds. This method, based on the Padé approximant, only requires real input in order to reconstruct the underlying function not only along the real axis but also in the complex plane within a certain radius of convergence. The method is universal being model independent, easy to use, and it has a broad range of applicability. We refer to this method as the Resonances Via Padé (RVP) method.

In order to demonstrate the abilities of this method we have applied it to several different situations. First, an analytical model for the spectral density function was studied and the resonance pole in the complex plane as well as two decay thresholds were correctly identified. Then, the method was applied to experimental data on the squared modulus of the pion form factor, $|F_\pi(s)|^2$, from which the resonance pole of the charged $\rho(770)$ meson was extracted in very good agreement with other predictions from the literature. In addition, we applied the RVP method to the real part of the partial wave amplitude in the

$IJ = 00$ channel of $\pi\pi$ scattering and extracted the resonance pole of the $f_0(500)$ - or σ meson, again in very good agreement with the most recent and precise determinations from the literature. Finally, we analyzed experimental data on the cross section ratio $R(s)$ from e^+e^- collisions and found that the extraction of decay thresholds is possible as long as the data are not too noisy or sparse.

We believe that this method does not only represent a viable tool to improve or supplement current determinations of resonance poles but that it can also be applied to a variety of other situations. In future applications we will further explore its potential and intend to use it, for example, to determine the temperature dependence of resonance poles for hadrons in a hot and dense medium or to obtain real-time correlation functions from their imaginary-time counterparts.

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